Supplementary Information (SI) for

Van der Waals heterostructures based on MSSe (M = Mo, W) and graphene-like GaN: Enhanced optoelectronic and photocatalytic properties for water splitting

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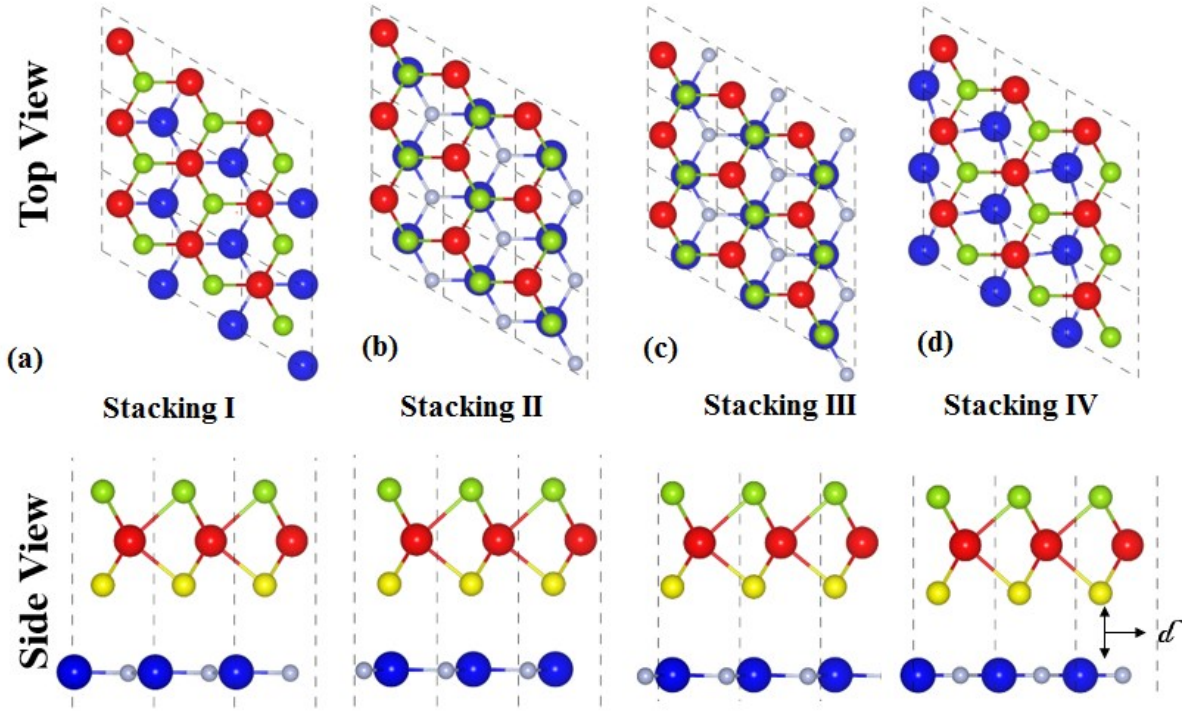

Fig. S1. The atomic structures of MSSe-g-GaN heterostructures for all stacking configurations of (a) stacking I, (b) stacking II, (c) stacking III and (d) stacking IV, respectively. The red, yellow and cyan balls stand for metal (Mo or W) and chalcogen (S or Se) atoms, respectively. The dard blue and gray balls represent the Ga and N atoms, respectively.

Tab. S1. Calculated binding energies and interlayer distance in the MSSe-g-GaN heterostructures for all stacking configurations of model I and model II.

Configurations	**Systems**	**MoSSe-GaN**		**WSSe-GaN**	
		(Model I)	**(Model II)**	**(Model I)**	**(Model II)**
Stacking I	Binding energy, eV	-0.38	-0.32	-0.30	-0.23
	Interlayer distance, Å	3.29	3.35	0.36	3.26
Stacking II	Binding energy, eV	-0.35	-0.39	-0.26	-0.29
	Interlayer distance, Å	0.31	0.30	3.36	3.18
Stacking III	Binding energy, eV	-0.40	-0.35	-0.21	-0.26
	Interlayer distance, Å	3.23	3.33	3.40	3.22
Stacking IV	Binding energy, eV	-0.48	-0.41	-0.35	-0.32
	Interlayer distance, Å	3.0	3.02	2.95	3.05